Effects of cross sections tables generation and optimization on rod ejection transient analyses

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A B S T R A C T

Best estimate analysis of rod ejection transients requires 3D kinetics core simulators. If they use cross sections libraries compiled in multidimensional tables, interpolation errors – originated when the core simulator computes the cross sections from the table values – are a source of uncertainty in k-effective calculations that should be accounted for. Those errors depend on the grid covering the domain of state variables and can be easily reduced, in contrast with other sources of uncertainties such as the ones due to nuclear data, by choosing an optimized grid distribution.

The present paper assesses the impact of the grid structure on a PWR rod ejection transient analysis using the coupled neutron-kinetics/thermal-hydraulics COBAYA3/COBRA-TF system. For this purpose, the OECD/NEA PWR MOX/UO_2 core transient benchmark has been chosen, as material compositions and geometries are available, allowing the use of lattice codes to generate libraries with different grid structures.

Since a complete nodal cross-section library is also provided as part of the benchmark specifications, the effects of the library generation on transient behavior are also analyzed. Results showed large discrepancies when using the benchmark library and own-generated libraries when compared with benchmark participants' solutions. The origin of the discrepancies was found to lie in the nodal cross sections provided in the benchmark.

1. Introduction

An accurate analysis of most LWR transients requires coupled neutronics/thermal-hydraulics calculations based on 3D kinetics methods. It is the case of main steam line break events (Ivanov et al., 1999) or rod ejection scenarios (Kozlowski and Downar, 2003), where the strongly asymmetric redistribution of the neutron flux cannot be studied using point kinetics methods. The 3D kinetics core simulators available nowadays to perform those best estimate analyses are based on few-group diffusion theory, which employs as input data pregenerated homogenized macroscopic cross sections compiled in libraries.

In addition to the interest in LWR best estimate predictions, in recent years there has been an increasing concern for the identification of the sources of uncertainties along with the quantification of their impact on coupled neutronics/thermal-hydraulics simulations (Ivanov et al., 2012). Understanding these sources is important to introduce appropriate design margins in safety analysis and decide where additional efforts should be undertaken to reduce uncertainties.

Neutronics-related uncertainties are one of the main contributors when modeling LWR transients and need to be evaluated. If 3D kinetics simulators are used, those uncertainties arise not only from the uncertainties in basic nuclear data, but also from the ones associated with methods and modeling approximations utilized, first, to derivate multigroup microscopic cross sections libraries through *cell physics* codes; second, to produce few group macroscopic cross sections libraries through *lattice physics* codes; and finally, to extract the cross sections values in the 3D *core physics* simulators.

In particular, if the few group macroscopic cross sections libraries are compiled in a multidimensional tabulated form, the interpolation errors, when computing the cross sections from the table values during the core calculation, are one source of uncertainties to be considered. Once the feedback variables have been chosen, interpolation errors depend on the mesh structure covering the expected variables' range, as well as the employed interpolation algorithm.

In a previous work (Sánchez-Cervera et al., 2014) we demonstrated, by performing 2D fuel assembly diffusion calculations with COBAYA3 code (Herrero, 2012), that the interpolation of cross sections is a non-negligible source of uncertainties in k-effective calculations. Then, we proposed a procedure to optimize cross

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sections tabulated libraries, showing that those uncertainties can be reduced by choosing an adequate mesh point distribution for the feedback variables, so that the cross sections interpolation errors have an impact on k-effective lower than a target value fixed by the user. A linear interpolation algorithm was chosen, since it is simple to implement and diffusion codes usually employ it during the whole core calculation.

The first objective of the present paper is to assess the impact of the grid point distribution, and therefore of the interpolation errors, on a best estimate rod ejection transient analysis at core level. For this purpose, the OECD/NEA PWR MOX/UO_2 core transient benchmark (Kozlowski and Downar, 2003) was selected.

In the benchmark, material compositions and pin geometries are provided, so it is possible to use a lattice physics code to generate new libraries with different grid point distributions. Additionally, a two group library at the nodal level is available for a given mesh of feedback variables. Consequently, a second objective of the paper is to assess the effects of the library generation on transient results, by comparison with the solutions submitted by benchmark participants and reported in (Kozlowski and Downar, 2007).

The following section briefly summarizes the specifications of the rod ejection transient benchmark. Different tabulated libraries are presented in Section 3, while Section 4 includes the results of the benchmark using each of those libraries. Conclusions are discussed in the final section.

2. Specifications for a rod ejection transient benchmark

The PWR MOX/UO_2 core transient benchmark was designed to assess the ability of modern reactor kinetics codes to model rod ejection transients and predict the transient response of a core partially loaded with MOX fuel. This event is of particular concern for MOX fueled cores because of the smaller delayed neutron fraction with respect to UO_2 cores.

The core is based on a 3565 MW_{th} four-loop Westinghouse PWR power plant with 193 fuel assemblies. Its configuration is shown in Fig. 1, corresponding to a three-batch equilibrium cycle. The core has uniform fuel composition in axial direction. The benchmark is composed of four different exercises, being Parts III and IV the ones computed for this paper:

- Part III is devoted to compute a 3D HZP steady state, being the coolant inlet temperature and pressure 560 K and 15.5 MPa. Control banks are fully inserted, while shutdown banks are completely withdrawn. A critical boron concentration search is to be performed.
- In Part IV, starting from the previous steady state conditions, a rod is assumed to be fully ejected in 0.1 s after which no reactor scram is considered. During the entire calculation, the boron concentration and the position of the other control rods are assumed to be constant. The transient is to be calculated for 1.0 s.

3. Cross sections libraries used

In the benchmark, all necessary few-group constants at the level of homogenized assembly were provided as a part of the benchmark specifications. Additionally, the benchmark also specifies material compositions and pin geometries so that participants can utilize other lattice physics codes to generate their own cross sections. This makes the benchmark suitable for the purpose of this work, where the effects of different cross sections libraries on transient results are to be assessed. Three libraries were used, as defined in the following.

3.1. Cross sections library provided in the benchmark (LIB-A)

A complete tabulated library with 2 group macroscopic cross sections and kinetic parameters for each assembly type is provided in the NEMTAB format used for the OECD MSLB benchmark (Ivanov et al., 1999). The two group structure uses the standard 0.625 eV energy cutoff. Let us refer this library as LIB-A from now on.

The cross sections were calculated with HELIOS1.7 lattice code (Giust et al., 2001) with a 47 group library at different conditions

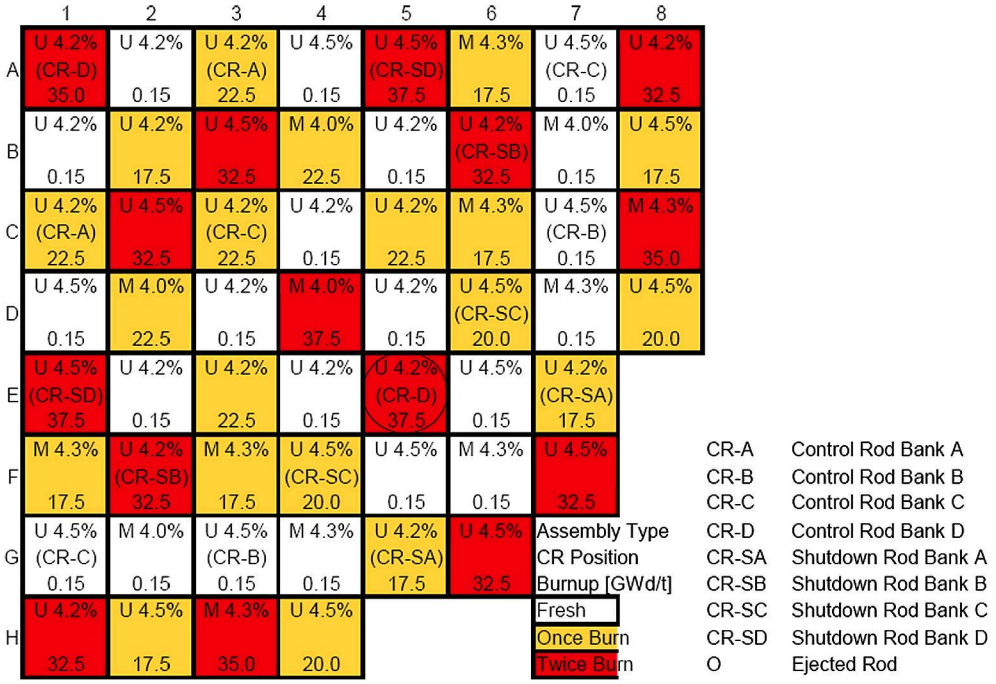

Fig. 1. Core configuration.

for fuel temperatures, moderator densities and boron concentrations to cover the expected range of core operating conditions.

Here, the moderator temperature is not included as a state variable, but its effect is treated implicitly in the moderator density assuming single phase at constant pressure. Control rod is not taken as state variable but the same branch calculations performed without control rod are made with the control rod inserted.

The conditions for the branch calculations are shown in Table 1, where a mesh with three different data points per state variable was considered, and a total of 27 branch calculations were performed for each assembly type.

3.2. Generated cross sections library using the benchmark state points mesh (LIB-B)

Starting from the geometry and number densities provided in the benchmark specifications, a 2 group library in the same NEMTAB format was produced using APOLLO2.8 lattice code (Sánchez, 1998 and Santamarina et al., 2013) and referred to as library LIB-B. The same mesh with three data points per state variable specified in the benchmark library was considered here, as indicated in Table 2. Therefore, the difference between LIB-A and LIB-B is the lattice code and multigroup library used for the cross sections generation.

It is possible to assess the influence that the cross sections interpolation errors will have in k-effective in 2D single assembly diffusion calculations when using this mesh. Let us consider the midpoints of the mesh for each state variable and compute the exact cross sections values with APOLLO2. The error in k-effective at those midpoints due to error contributions from all cross sections will be the difference between the k-effective computed with the exact cross sections and the one computed using the interpolated values.

Proceeding this way, the maximum error found in k-effective per state variable was 37 pcm. As a consequence, the combination of errors in 3D coupled neutronics/thermal-hydraulics calculations would induce a higher k-effective error.

3.3. Generated cross sections library using an optimized state points mesh (LIB-C)

An additional library, referred as LIB-C, was produced starting from the geometry and number densities using APOLLO2.8 lattice code, but considering an optimized mesh. Therefore, the difference between LIB-B and LIB-C is only the number and distribution of the grid points in the tabulated library.

The optimized mesh has been obtained following the method described in (Sánchez-Cervera et al., 2014). Optimality is considered in the sense of building an interpolation grid with the minimum number of grid points per state variable, satisfying a user given target accuracy in the computed k-effective. The optimization procedure is based on the computation of the sensitivity coefficients of k relative to the cross sections using adjoint sensitivity analysis (ASAP) in the COBAYA3 code. Sensitivity coefficients play a major role since allow evaluating the influence of interpolation errors on k-effective. Then, it is possible to find a relationship between the k-effective error and the positions of the grid points.

In (Sánchez-Cervera et al., 2014), the optimization process was illustrated for fuel assemblies defined in this same benchmark, imposing different levels of accuracy in k-effective. The optimal multidimensional point distribution was found to be very similar for assemblies of the same type but different enrichment and burnup. However, differences were found for MOX fuel assemblies. Also, a broader variation range for the state variables was defined, since a general library applicable to cases with moderator boiling was pursued.

For the present work, the variation domain for the state variables is the one defined in the benchmark, and a level of accuracy in k of 5 pcm per state variable was selected. The optimal grid structures were built for the UO_2 and MOX fuel assemblies, the latter imposing the most restrictive mesh, shown in Table 3, and considered for generating the whole library. It can be noticed how different the level of mesh refinement required for each state variables is; e.g. optimum grid for fuel temperature contains much more data points that the one for moderator density.

Table 1
Lattice code and cross sections branch points for the library provided in the benchmark (LIB-A).

Lattice code used: HELIOS1.7 – 47G library			
Fuel temperature (K)	560	900	1320
Boron concentration (ppm)	0	1000	2000
Moder. density (kg/m^3)	661.14	711.87	752.06

Table 2
Lattice code and cross section branch model for the generated library using the benchmark mesh (LIB-B).

Lattice code used: APOLLO2.8 – 281G based JEFF3.1.1 library			
Fuel temperature (K)	560	900	1320
Boron concentration (ppm)	0	1000	2000
Moder. density (kg/m^3)	661.14	711.87	752.06

4. Benchmark results

The benchmark analysis has been performed using the ANDES solver of COBAYA3, which is a nodal diffusion code, coupled to the COBRA-TF thermal-hydraulics code. First, it has been computed using LIB-A, and then, repeated with the two additional libraries, LIB-B and LIB-C. Results have been compared with the solutions submitted by benchmark participants.

4.1. Results of Part III. 3D HZP steady state

Several benchmark participants submitted solutions for Part III with few-group nodal diffusion methods, such as CORETRAN (Eisenhart et al., 2000) or PARCS (Downar et al., 2002), and with the multigroup homogeneous transport code BARS (Akimushkin et al., 2002) and the heterogeneous transport code DeCART (Joo et al., 2002). Since the nodal cross-sections were generated using HELIOS with a 47-group library, and DeCART library is based on the same 47-group library, DeCART can be taken as the reference solution as its transport calculation includes the most accurate method and the most detailed description of the core.

A comparison of critical boron concentration and assembly power is shown in Table 4, where the results obtained with COBAYA3 using LIB-A, LIB-B and LIB-C are also included. To evaluate the assembly power errors, the power-weighted error (PWE) and error-weighted error (EWE) defined in the final benchmark report (Kozlowski and Downar, 2007) are used. The PWE is similar to absolute error, but it weights the per cent error with the reference power; the EWE weights the largest per cent errors more than the small ones.

The agreement between nodal methods is excellent when using the same benchmark library, LIB-A, and the same mesh of four nodes per fuel assembly. Differences lower than 5 ppm in critical boron concentration and 0.0% and 0.3% in the radial and axial peaking factors were found between COBAYA3 and PARCS. A more detailed comparison, e.g. effects of different nodalizations, or

Table 3
Lattice code and cross sections branch points for the generated library using the optimized mesh (LIB-C).

Lattice code used: APOLLO2.8 – 281G based JEFF3.1.1 library								
Fuel temperature (K)	560	640	720	850	950	1070	1200	1348
Boron concentration (ppm)	0	325	833	1452	2106	–	–	–
Moder. density (kg/m^3)	661.14	715.5	772	836	–	–	–	–

Table 4
Comparison of critical boron and assembly power errors for Part III.

Code	Solution method	Library	Critical boron (ppm)	Assembly power error	
				% PWE	% EWE
DeCART	Pin heterogeneous MOC transport	47G based on HELIOS 1.8 library	1265	Ref	Ref
BARS	Pin homogeneous lambda matrix	5G library from UNK	1296	2.65	5.66
PARCS	Nodal diffusion (4 N/FA)	2G nodal LIB-A from HELIOS 1.7	1341	1.05	3.49
CORETRAN	Nodal diffusion (4 N/FA)	2G nodal LIB-A from HELIOS 1.7	1346	1.09	3.72
COBAYA3	Nodal diffusion (4 N/FA)	2G nodal LIB-A from HELIOS 1.7	1345	1.06	3.24
COBAYA3	Nodal diffusion (4 N/FA)	2G nodal LIB-B from APOLLO2	1292	1.70	4.02
COBAYA3	Nodal diffusion (4 N/FA)	2G nodal LIB-C from APOLLO2	1269	1.49	4.19

number of energy groups can be found in (Lozano et al., 2008). However, a non-negligible difference can be found in the critical boron concentration computed by the nodal codes using the benchmark library with respect to the solutions provided by the codes BARS and DeCART.

If COBAYA3 results are computed using the new library LIB-B, the critical boron concentration is about 50 ppm lower, and the agreement with BARS and DeCART boron prediction is noticeably improved. Power distributions become closer to BARS and, consequently, PWE and EWE errors increase slightly with respect to DeCART reference solution.

The Russian Kurchatov Institute was the only benchmark participant producing their own library from the provided nuclide densities suitable to perform calculations with BARS. They reported to produce a 5 energy groups library generated with UNK lattice code using ENDF/B-VI. Agreement between COBAYA3 using LIB-B and BARS is very good, even if discrepancies were expected due to the different multigroup libraries employed, approximations in the used lattice codes, and transport approximation methods in the core simulators.

Finally, results obtained with COBAYA3 using the optimized mesh (LIB-C) show the benefits of the optimization process, since the mesh refinement employed yields almost the same boron concentration that DeCART. Power distributions are very similar to the ones predicted by BARS, with relative differences lower than 0.1%.

In summary, the primary reason for the discrepancies between the benchmark participants in Part III is the neutron nodal cross sections library, and no other aspects such as the accuracy of the 3D kinetics solvers used for the core calculation. Calculations performed by APOLLO2/COBAYA3 suggest that either the nuclide densities, or geometries, or the transport calculation options employed to produce the cross sections libraries are not in agreement with the ones used in HELIOS to produce the benchmark libraries (e.g. different reduction of isotopes with low densities, simplifications made in the specifications and not considered in HELIOS, ...).

4.2. Results of Part IV. Rod ejection 3D transient

Regarding Part IV of the benchmark, all nodal codes provided solutions, but for the higher order transport codes, only BARS submitted results, since some limitations prevented DeCART from computing a reference solution. The predicted transient behavior is compared in Fig. 2, and values of maximum reactivity, peak power, peak time and Doppler temperature are given in Table 5. The results obtained with COBAYA3/COBRA-TF using LIBS A, B and C are also included.

Results show that all nodal diffusion codes provide very similar solutions when using the same cross sections library, with some differences due to the employed nodal method and/or the NK/TH solution scheme.

However, the BARS transport solution is significantly different to the rest. In the benchmark final report, differences in BARS were explained as a consequence of the different radial and axial power shape predicted in Part III, attributed to the neutron cross sections, but it could not be totally resolved.

Now, comparison between COBAYA3/COBRA-TF results when using LIB-A and LIB-B also shows these same discrepancies. When using the recomputed library, COBAYA3 predicts a peak power about three times higher and a power excursion earlier than when using the benchmark library, yielding thereby a peak power and a time of power maximum closer to the BARS solution. That is, the nodal cross sections specified in the benchmark do not agree with the specifications to generate own libraries as employed by BARS.

The justification for those two main differences (the peak value and the earlier peak time) relies on the cross sections libraries. Firstly, different values of the cross sections for the controlled assembly in position E-5 in Fig. 1 yield to different values of reactivity insertion when that rod is ejected. Secondly, different kinetics parameters in LIB-A and LIB-B can be found. For example, while LIB-A considers the same values of $1/v$ for rodded and unrodded assemblies and no parameterization with state variables, LIB-B provides different values of $1/v$ for each type of assembly and for each combination of state variables.

For the purpose of assessing the effect of the cross sections table optimization on the rod ejection transient, the results with COBAYA3 using the optimized library, LIB-C, show that the core power evolution with the optimized mesh is quite similar to the one predicted using the benchmark mesh, LIB-B, although the peak power value decreases 7% with the mesh refinement.

5. Conclusions

In this paper, the impact of the generation and optimization of nodal cross sections libraries on the OECD/NEA PWR MOX/UO_2 PWR rod ejection transient benchmark is assessed. Three different cross sections libraries were used to perform the transient calculations using the coupled neutron-kinetics/thermal-hydraulics COBAYA3/COBRA-TF system: the benchmark library (LIB-A), a newly generated library with the same benchmark mesh for the

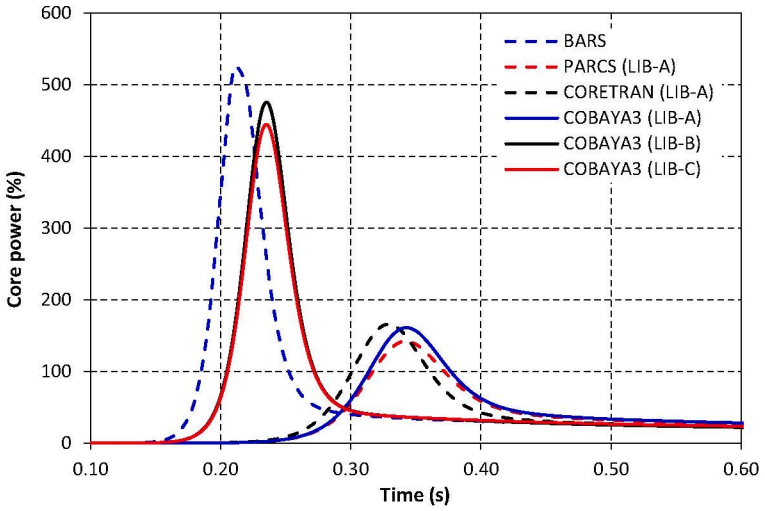

Fig. 2. Evolution of core power during the rod ejection transient.

Table 5
Comparison of transient solutions computed for Part IV.

Code	Library	Peak time (s)	Peak power (MW)	Peak power (%)	Maximum reactivity (pcm)	T_{Dop} (t = 1 s) (K)
BARS	UNK 5G library	0.21	18,607	522	1.29	597
PARCS	2G nodal LIB-A	0.34	5052	142	1.12	582
CORETRAN	2G nodal LIB-A	0.33	5926	166	1.14	586
COBAYA3	2G nodal LIB-A	0.34	5725	161	1.11	583
COBAYA3	2G nodal LIB-B	0.23	16,955	475	1.15	591
COBAYA3	2G nodal LIB-C	0.23	15,847	444	1.15	591

state variables (LIB-B) and other newly generated library with an optimized mesh (LIB-C).

The steady state prior to the transient was computed and results compared with transport solutions submitted by benchmark participants. The agreement of COBAYA3 critical boron concentration was clearly improved when using LIB-B and especially LIB-C, with respect to using LIB-A. However, with those new libraries, assembly power distributions were found to be more similar to BARS solution than to DeCART reference solution.

Rod ejection transient results obtained with LIB-A also showed large differences against results computed with LIB-B and LIB-C. With those new libraries, the power excursion occurs earlier and the peak power prediction is about three times higher, being the agreement with BARS solution noticeably improved. The mesh optimization (LIB-C) had an effect of decreasing the peak power value by 7% while the peak maximum was reached at the same instant than solution provided using LIB-B.

Results show that the origin of the discrepancies in the final benchmark report between nodal and transport solutions lies in the nodal cross sections provided in the benchmark, which are not consistent with the material compositions and/or geometry specifications and hypothesis contained in the specification.

Optimization process led to a more refined mesh, so it was demonstrated here that an adequate refinement of the grid mesh has an important effect on transient results. That is, interpolation errors are a non-negligible source of uncertainties in the solution and their influence has to be accounted for in best estimate analysis. Those uncertainties can be reduced by optimizing the grid point distribution satisfying a target accuracy given by the user.

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